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Solvophobic effects: Qualitative determination and quantitative description

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Abstract

Solvophobic effects strongly influence the thermodynamic properties of solutions and are one of the driving forces of self-assembly processes of supramolecular structures. However, the generally accepted definition and a quantitative measure of these effects have so far been absent. Based on the analysis of a large set of experimental data on the thermodynamic functions of solvation in various systems, we propose a qualitative criterion allowing us to judge about whether the solvophobic effects are manifested in the solution or not, and also a method to determine their contributions to the thermodynamic functions of solvation. A feature of the solvophobic effect is a violation of the linear relationship between the Gibbs free energy and the enthalpy of solvation, which is fulfilled for the solutions of different compounds in many non-associated solvents. It is shown that in self-associated solvents the solvophobic effect is observed for any dissolved compounds, including well soluble ones, resulting in an increase in the Gibbs energy of solvation. Previously proposed solvophobicity parameters are considered and compared with our results.

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Keywords

Enthalpy, Gibbs free energy, Self-association, Solvophobic effects